



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:52 AM GMT

PDB ID : 3N2B  
Title : 1.8 Angstrom Resolution Crystal Structure of Diaminopimelate Decarboxylase (lysA) from *Vibrio cholerae*.  
Authors : Minasov, G.; Halavaty, A.; Shuvalova, L.; Dubrovskaya, I.; Winsor, J.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-05-17  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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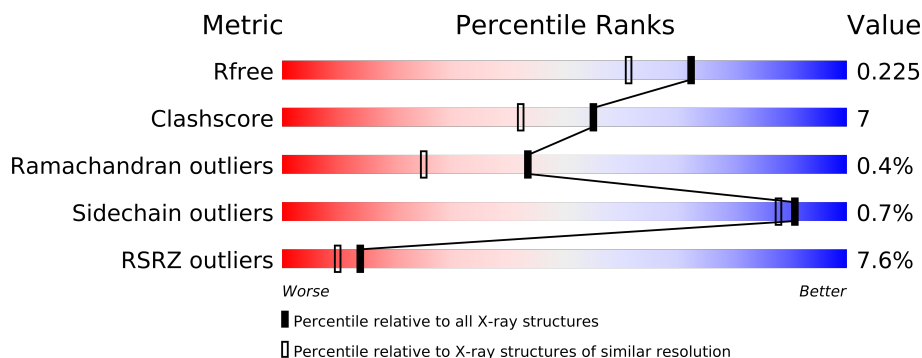
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	441	
1	B	441	
1	C	441	
1	D	441	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14009 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	8	0
			3279	2072	579	618	10			
1	B	392	Total	C	N	O	S	0	7	0
			3123	1982	546	586	9			
1	C	411	Total	C	N	O	S	0	10	0
			3283	2079	574	620	10			
1	D	398	Total	C	N	O	S	0	8	0
			3179	2008	558	603	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP Q9KVL7
A	-22	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-21	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-20	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-19	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-18	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-17	HIS	-	EXPRESSION TAG	UNP Q9KVL7
A	-16	SER	-	EXPRESSION TAG	UNP Q9KVL7
A	-15	SER	-	EXPRESSION TAG	UNP Q9KVL7
A	-14	GLY	-	EXPRESSION TAG	UNP Q9KVL7
A	-13	VAL	-	EXPRESSION TAG	UNP Q9KVL7
A	-12	ASP	-	EXPRESSION TAG	UNP Q9KVL7
A	-11	LEU	-	EXPRESSION TAG	UNP Q9KVL7
A	-10	GLY	-	EXPRESSION TAG	UNP Q9KVL7
A	-9	THR	-	EXPRESSION TAG	UNP Q9KVL7
A	-8	GLU	-	EXPRESSION TAG	UNP Q9KVL7
A	-7	ASN	-	EXPRESSION TAG	UNP Q9KVL7
A	-6	LEU	-	EXPRESSION TAG	UNP Q9KVL7
A	-5	TYR	-	EXPRESSION TAG	UNP Q9KVL7
A	-4	PHE	-	EXPRESSION TAG	UNP Q9KVL7
A	-3	GLN	-	EXPRESSION TAG	UNP Q9KVL7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KVL7
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KVL7
A	0	ALA	-	EXPRESSION TAG	UNP Q9KVL7
B	-23	MET	-	EXPRESSION TAG	UNP Q9KVL7
B	-22	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-21	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-20	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-19	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-18	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-17	HIS	-	EXPRESSION TAG	UNP Q9KVL7
B	-16	SER	-	EXPRESSION TAG	UNP Q9KVL7
B	-15	SER	-	EXPRESSION TAG	UNP Q9KVL7
B	-14	GLY	-	EXPRESSION TAG	UNP Q9KVL7
B	-13	VAL	-	EXPRESSION TAG	UNP Q9KVL7
B	-12	ASP	-	EXPRESSION TAG	UNP Q9KVL7
B	-11	LEU	-	EXPRESSION TAG	UNP Q9KVL7
B	-10	GLY	-	EXPRESSION TAG	UNP Q9KVL7
B	-9	THR	-	EXPRESSION TAG	UNP Q9KVL7
B	-8	GLU	-	EXPRESSION TAG	UNP Q9KVL7
B	-7	ASN	-	EXPRESSION TAG	UNP Q9KVL7
B	-6	LEU	-	EXPRESSION TAG	UNP Q9KVL7
B	-5	TYR	-	EXPRESSION TAG	UNP Q9KVL7
B	-4	PHE	-	EXPRESSION TAG	UNP Q9KVL7
B	-3	GLN	-	EXPRESSION TAG	UNP Q9KVL7
B	-2	SER	-	EXPRESSION TAG	UNP Q9KVL7
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KVL7
B	0	ALA	-	EXPRESSION TAG	UNP Q9KVL7
C	-23	MET	-	EXPRESSION TAG	UNP Q9KVL7
C	-22	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-21	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-20	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-19	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-18	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-17	HIS	-	EXPRESSION TAG	UNP Q9KVL7
C	-16	SER	-	EXPRESSION TAG	UNP Q9KVL7
C	-15	SER	-	EXPRESSION TAG	UNP Q9KVL7
C	-14	GLY	-	EXPRESSION TAG	UNP Q9KVL7
C	-13	VAL	-	EXPRESSION TAG	UNP Q9KVL7
C	-12	ASP	-	EXPRESSION TAG	UNP Q9KVL7
C	-11	LEU	-	EXPRESSION TAG	UNP Q9KVL7
C	-10	GLY	-	EXPRESSION TAG	UNP Q9KVL7
C	-9	THR	-	EXPRESSION TAG	UNP Q9KVL7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	EXPRESSION TAG	UNP Q9KVL7
C	-7	ASN	-	EXPRESSION TAG	UNP Q9KVL7
C	-6	LEU	-	EXPRESSION TAG	UNP Q9KVL7
C	-5	TYR	-	EXPRESSION TAG	UNP Q9KVL7
C	-4	PHE	-	EXPRESSION TAG	UNP Q9KVL7
C	-3	GLN	-	EXPRESSION TAG	UNP Q9KVL7
C	-2	SER	-	EXPRESSION TAG	UNP Q9KVL7
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KVL7
C	0	ALA	-	EXPRESSION TAG	UNP Q9KVL7
D	-23	MET	-	EXPRESSION TAG	UNP Q9KVL7
D	-22	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-21	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-20	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-19	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-18	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-17	HIS	-	EXPRESSION TAG	UNP Q9KVL7
D	-16	SER	-	EXPRESSION TAG	UNP Q9KVL7
D	-15	SER	-	EXPRESSION TAG	UNP Q9KVL7
D	-14	GLY	-	EXPRESSION TAG	UNP Q9KVL7
D	-13	VAL	-	EXPRESSION TAG	UNP Q9KVL7
D	-12	ASP	-	EXPRESSION TAG	UNP Q9KVL7
D	-11	LEU	-	EXPRESSION TAG	UNP Q9KVL7
D	-10	GLY	-	EXPRESSION TAG	UNP Q9KVL7
D	-9	THR	-	EXPRESSION TAG	UNP Q9KVL7
D	-8	GLU	-	EXPRESSION TAG	UNP Q9KVL7
D	-7	ASN	-	EXPRESSION TAG	UNP Q9KVL7
D	-6	LEU	-	EXPRESSION TAG	UNP Q9KVL7
D	-5	TYR	-	EXPRESSION TAG	UNP Q9KVL7
D	-4	PHE	-	EXPRESSION TAG	UNP Q9KVL7
D	-3	GLN	-	EXPRESSION TAG	UNP Q9KVL7
D	-2	SER	-	EXPRESSION TAG	UNP Q9KVL7
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KVL7
D	0	ALA	-	EXPRESSION TAG	UNP Q9KVL7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	C	2	Total Cl 2 2	0	0

- Molecule 3 is water.

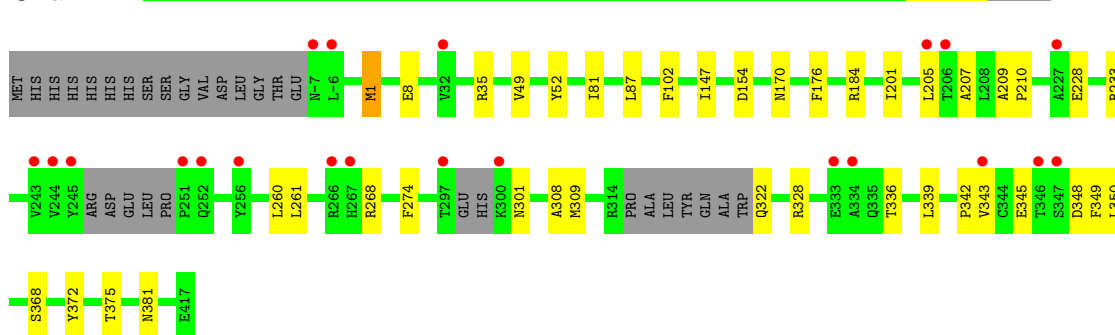
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	324	Total 328	O 328	0	5
3	B	280	Total 284	O 284	0	4
3	C	285	Total 290	O 290	0	7
3	D	232	Total 239	O 239	0	7

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

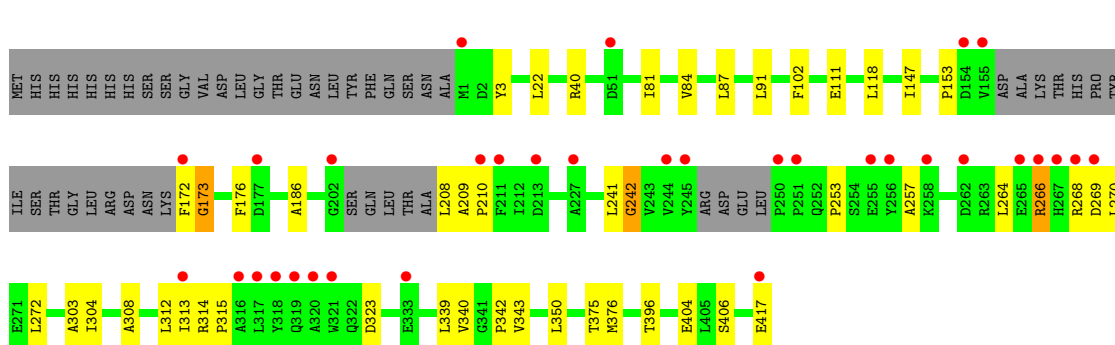
- Molecule 1: Diaminopimelate decarboxylase

Chain A:



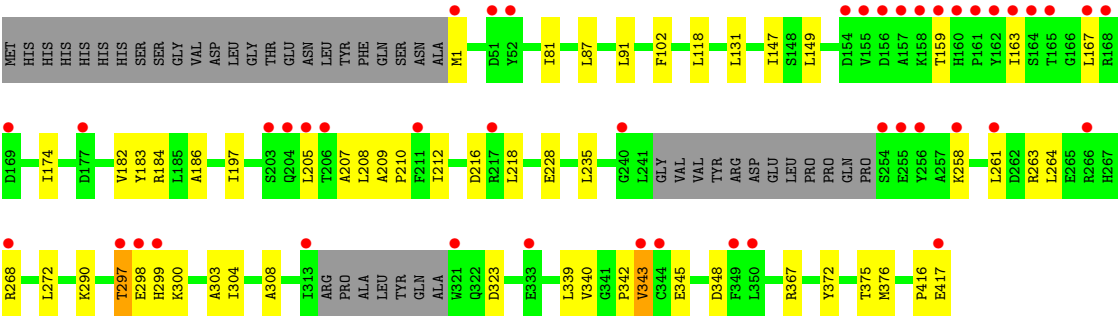
- Molecule 1: Diaminopimelate decarboxylase

Chain B:



● Molecule 1: Diaminopimelate decarboxylase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.39Å 80.33Å 118.69Å 105.31° 93.62° 90.52°	Depositor
Resolution (Å)	29.94 – 1.80 29.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.94-1.80) 97.5 (29.83-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.183 , 0.219 0.189 , 0.225	Depositor DCC
$R_{free}$ test set	7289 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 145780 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	0/3340	0.68	0/4521
1	B	0.56	0/3185	0.69	1/4317 (0.0%)
1	C	0.54	0/3352	0.68	0/4543
1	D	0.54	0/3239	0.68	0/4388
All	All	0.56	0/13116	0.68	1/17769 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	GLY	N-CA-C	5.05	125.72	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3279	0	3261	40	0
1	B	3123	0	3101	34	0
1	C	3283	0	3260	40	0
1	D	3179	0	3152	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	328	0	0	1	0
3	B	284	0	0	4	0
3	C	290	0	0	2	0
3	D	239	0	0	3	0
All	All	14009	0	12774	171	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233[B]:ARG:HG2	1:A:233[B]:ARG:NH2	1.58	1.05
1:A:233[B]:ARG:CG	1:A:233[B]:ARG:HH21	1.74	0.99
1:A:233[B]:ARG:HG2	1:A:233[B]:ARG:HH21	0.84	0.98
1:A:343:VAL:HG13	1:A:381:ASN:OD1	1.64	0.97
1:A:308:ALA:HB1	1:A:343:VAL:HG23	1.50	0.93
1:C:264:LEU:HD13	1:C:272:LEU:HD11	1.50	0.92
1:B:304:ILE:HD13	1:B:340:VAL:CG2	2.02	0.90
1:A:343:VAL:HG12	1:A:345:GLU:HG2	1.58	0.85
1:C:91[B]:LEU:HD11	1:C:118:LEU:CD1	2.09	0.82
1:D:268[B]:ARG:H	1:D:268[B]:ARG:NE	1.80	0.80
1:A:308:ALA:HB1	1:A:343:VAL:CG2	2.13	0.79
1:D:268[B]:ARG:HE	1:D:268[B]:ARG:H	1.31	0.79
1:D:298:GLU:HB2	1:D:299:HIS:HA	1.65	0.77
1:B:304:ILE:HD13	1:B:340:VAL:HG23	1.66	0.76
1:B:91[A]:LEU:HD11	1:B:118:LEU:HD13	1.67	0.76
1:C:264:LEU:CD1	1:C:272:LEU:HD11	2.14	0.76
1:A:308:ALA:HB2	1:A:342:PRO:HD2	1.67	0.75
1:C:91[B]:LEU:HD11	1:C:118:LEU:HD13	1.68	0.75
1:D:304:ILE:HD13	1:D:340:VAL:CG2	2.17	0.75
1:C:264:LEU:HD13	1:C:272:LEU:HD21	1.67	0.75
1:D:218:LEU:HD21	1:D:235:LEU:HD11	1.69	0.74
1:A:8[B]:GLU:CD	1:A:8[B]:GLU:O	2.27	0.73
1:B:147:ILE:HD11	1:B:186:ALA:HB1	1.72	0.71
1:D:343:VAL:HG22	1:D:348:ASP:OD2	1.91	0.71
1:D:304:ILE:HD13	1:D:340:VAL:HG23	1.74	0.69
1:D:297:THR:HB	1:D:298:GLU:HA	1.73	0.69
1:B:268:ARG:CB	1:B:269:ASP:HA	2.23	0.69
1:D:297:THR:HG22	1:D:298:GLU:O	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:THR:HG23	3:B:520:HOH:O	1.91	0.69
1:C:331[B]:GLN:OE1	1:C:332:GLY:N	2.26	0.68
1:A:8[B]:GLU:C	1:A:8[B]:GLU:OE2	2.34	0.66
1:B:268:ARG:HB3	1:B:269:ASP:HA	1.79	0.64
1:D:208:LEU:HD21	1:D:212:ILE:HD11	1.80	0.64
1:D:147:ILE:HD11	1:D:186:ALA:HB1	1.78	0.64
1:C:264:LEU:CD1	1:C:272:LEU:HD21	2.27	0.64
1:D:174:ILE:HD13	1:D:182:VAL:HG21	1.79	0.64
1:C:91[B]:LEU:HD11	1:C:118:LEU:HD11	1.81	0.62
1:A:268:ARG:O	1:A:268:ARG:HG2	1.99	0.62
1:B:91[A]:LEU:HD11	1:B:118:LEU:CD1	2.29	0.61
1:B:304:ILE:CD1	1:B:340:VAL:HG23	2.31	0.61
1:D:91:LEU:HD11	1:D:118:LEU:CD1	2.31	0.61
1:D:208:LEU:O	1:D:208:LEU:HD23	2.01	0.60
1:D:290:LYS:HE3	3:D:524:HOH:O	2.01	0.60
1:C:264:LEU:HD13	1:C:272:LEU:CD1	2.26	0.60
1:B:304:ILE:CD1	1:B:340:VAL:CG2	2.77	0.60
1:C:308:ALA:HB2	1:C:342:PRO:HD2	1.84	0.59
1:A:1:MET:HA	1:A:1:MET:HE2	1.84	0.59
1:D:81:ILE:HD13	1:D:87:LEU:HB2	1.85	0.58
1:B:264:LEU:CD1	1:B:272:LEU:HD21	2.33	0.58
1:D:261:LEU:HD23	1:D:261:LEU:O	2.03	0.58
1:B:3:TYR:OH	1:B:40[A]:ARG:NH1	2.36	0.58
1:A:233[B]:ARG:CG	1:A:233[B]:ARG:NH2	2.43	0.58
1:C:174:ILE:CD1	1:C:182:VAL:HG11	2.34	0.58
1:C:268:ARG:HB3	1:C:269:ASP:HA	1.86	0.57
1:A:35:ARG:NH2	1:B:417:GLU:OE1	2.37	0.57
1:B:253:PRO:HB2	1:B:257:ALA:HB3	1.85	0.57
1:A:308:ALA:CB	1:A:343:VAL:HG23	2.30	0.57
1:C:147[A]:ILE:HD13	1:C:192:LEU:HD13	1.86	0.57
1:B:314:ARG:HB2	1:B:315:PRO:HD3	1.88	0.56
1:A:349:PHE:C	1:A:350:LEU:HD12	2.26	0.56
1:C:128:GLU:OE2	1:C:178:ARG:NH2	2.33	0.55
1:C:52:TYR:CE2	1:C:272:LEU:HG	2.40	0.55
1:A:8[B]:GLU:C	1:A:8[B]:GLU:CD	2.64	0.55
1:D:297:THR:HB	1:D:298:GLU:CA	2.35	0.55
1:C:303:ALA:HB3	1:C:339:LEU:HD13	1.88	0.55
1:A:201:ILE:HD11	1:A:260:LEU:HD22	1.89	0.55
1:D:303:ALA:HB3	1:D:339:LEU:HD13	1.89	0.54
1:C:174:ILE:HD13	1:C:182:VAL:HG11	1.90	0.54
1:C:343:VAL:HG22	1:C:348:ASP:OD2	2.07	0.53
1:A:343:VAL:N	1:A:348:ASP:OD2	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:304:ILE:CD1	1:D:340:VAL:HG23	2.38	0.53
1:C:196:GLY:HA2	1:C:232:ILE:HG23	1.92	0.52
1:D:159:THR:HG22	3:D:465:HOH:O	2.08	0.52
1:C:264:LEU:HD13	1:C:272:LEU:CD2	2.37	0.52
1:D:308:ALA:HB2	1:D:342:PRO:HD2	1.92	0.52
1:B:208:LEU:HD23	1:B:208:LEU:O	2.10	0.52
1:C:268:ARG:HA	1:C:270:LEU:H	1.75	0.52
1:D:339:LEU:HD22	1:D:339:LEU:N	2.25	0.52
1:D:91:LEU:HD11	1:D:118:LEU:HD11	1.93	0.51
1:D:208:LEU:HD21	1:D:212:ILE:CD1	2.39	0.51
1:D:163:ILE:O	1:D:167:LEU:HD13	2.10	0.51
1:A:81:ILE:HD13	1:A:87:LEU:HB2	1.92	0.51
1:C:266:ARG:HG3	1:C:267:HIS:N	2.26	0.51
1:A:309:MET:HG2	1:A:343:VAL:HG21	1.93	0.50
1:B:241:LEU:HB3	1:B:242:GLY:HA3	1.93	0.50
1:D:184:ARG:NE	1:D:228:GLU:OE2	2.38	0.50
1:B:264:LEU:HD11	1:B:272:LEU:HD21	1.92	0.50
1:B:308:ALA:HB2	1:B:342:PRO:HD2	1.94	0.50
1:B:81:ILE:HD13	1:B:87:LEU:HB2	1.94	0.50
1:D:264:LEU:HD11	1:D:272:LEU:HD21	1.94	0.50
1:C:45:PHE:HA	1:C:243:VAL:HG21	1.94	0.49
1:A:81:ILE:CD1	1:A:87:LEU:HB2	2.42	0.49
1:D:131:LEU:HD11	1:D:147:ILE:HD13	1.95	0.49
1:D:208:LEU:C	1:D:208:LEU:HD23	2.32	0.49
1:A:49[B]:VAL:HG11	1:A:274:PHE:CE2	2.49	0.48
1:D:216:ASP:OD1	1:D:263:ARG:HD3	2.13	0.48
1:A:49[A]:VAL:HG13	1:A:261:LEU:HD21	1.96	0.48
1:D:212:ILE:HG23	1:D:263:ARG:HD2	1.94	0.48
1:A:147:ILE:HD12	1:A:147:ILE:C	2.34	0.48
1:B:303:ALA:HB3	1:B:339:LEU:HD13	1.95	0.48
1:D:209:ALA:HB3	1:D:210:PRO:HD3	1.94	0.48
1:B:264:LEU:HD12	1:B:272:LEU:HD11	1.96	0.47
1:D:209:ALA:HB3	1:D:210:PRO:CD	2.44	0.47
1:D:375:THR:HG23	1:D:376:MET:HG3	1.96	0.47
1:D:298:GLU:HB2	1:D:299:HIS:CA	2.41	0.47
1:D:197:ILE:HG23	1:D:235:LEU:CD1	2.44	0.47
1:B:209:ALA:N	1:B:210:PRO:HD2	2.29	0.47
1:C:154:ASP:HB2	1:C:176:PHE:CG	2.50	0.47
1:D:208:LEU:CD2	1:D:212:ILE:CD1	2.92	0.47
1:B:84:VAL:HB	1:B:111:GLU:HG2	1.96	0.47
1:D:149:LEU:HD12	1:D:183:TYR:CD1	2.49	0.47
1:B:342:PRO:O	3:B:957:HOH:O	2.20	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:-2:SER:HA	1:C:5:ASN:ND2	2.29	0.47
1:A:1:MET:CE	1:A:1:MET:HA	2.44	0.47
1:A:350:LEU:HD12	1:A:350:LEU:N	2.30	0.46
1:A:339:LEU:N	1:A:339:LEU:HD12	2.30	0.46
1:D:264:LEU:CD1	1:D:272:LEU:HD21	2.45	0.46
1:B:268:ARG:HA	1:B:270:LEU:H	1.80	0.46
1:A:328:ARG:CZ	1:C:331[B]:GLN:HG2	2.46	0.45
1:A:154:ASP:HB2	1:A:176:PHE:CG	2.51	0.45
1:C:197:ILE:HB	1:C:232:ILE:HD13	1.98	0.45
1:D:218:LEU:HD21	1:D:235:LEU:CD1	2.43	0.45
1:A:209:ALA:HB3	1:A:210:PRO:CD	2.46	0.45
1:B:404[A]:GLU:OE2	1:B:406[A]:SER:OG	2.30	0.45
1:C:81:ILE:CD1	1:C:87:LEU:HB2	2.47	0.45
1:C:52:TYR:OH	1:C:267:HIS:O	2.29	0.44
1:D:304:ILE:CD1	1:D:340:VAL:CG2	2.90	0.44
1:C:234:HIS:CE1	3:C:441:HOH:O	2.69	0.44
1:A:301:ASN:HB2	1:A:336:THR:O	2.17	0.44
1:A:184:ARG:NE	1:A:228:GLU:OE1	2.34	0.44
1:D:205:LEU:HD12	1:D:205:LEU:N	2.32	0.44
1:D:372:TYR:HA	1:D:375:THR:CG2	2.47	0.44
1:D:91:LEU:HD11	1:D:118:LEU:HD13	1.98	0.44
1:D:323:ASP:HB3	1:D:367:ARG:HD3	1.98	0.44
1:B:323:ASP:OD1	3:B:951:HOH:O	2.21	0.43
1:A:343:VAL:CG1	1:A:345:GLU:HG2	2.38	0.43
1:A:268:ARG:CG	1:A:268:ARG:O	2.66	0.43
1:B:22:LEU:HD21	1:B:396:THR:HG21	2.00	0.43
1:B:266:ARG:H	1:B:266:ARG:CD	2.32	0.43
1:D:290:LYS:CE	3:D:524:HOH:O	2.65	0.43
1:B:312:LEU:HD23	1:B:350:LEU:HD22	2.01	0.43
1:C:313:ILE:HG23	1:C:313:ILE:O	2.19	0.42
1:D:343:VAL:CG2	1:D:348:ASP:OD2	2.63	0.42
1:D:197:ILE:HG23	1:D:235:LEU:HD12	2.01	0.42
1:C:268:ARG:HA	1:C:270:LEU:N	2.33	0.42
1:C:339:LEU:HD22	1:C:339:LEU:N	2.35	0.42
1:B:313:ILE:HG22	3:B:949:HOH:O	2.20	0.42
1:C:205:LEU:HD22	1:C:210:PRO:HB2	2.01	0.42
1:C:233:ARG:O	1:C:270:LEU:HA	2.20	0.42
1:B:153:PRO:HA	1:B:176:PHE:HE1	1.85	0.41
1:D:345:GLU:HB2	1:D:348:ASP:HB2	2.01	0.41
1:D:416:PRO:O	1:D:417:GLU:HB2	2.20	0.41
3:C:515:HOH:O	1:D:297:THR:HG22	2.19	0.41
1:C:252:GLN:HB2	1:C:253:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:ALA:HB1	3:A:576[B]:HOH:O	2.20	0.41
1:A:322:GLN:HG2	1:A:368[B]:SER:OG	2.21	0.41
1:A:372:TYR:HA	1:A:375:THR:CG2	2.50	0.41
1:D:268[A]:ARG:HA	1:D:268[A]:ARG:HD3	1.80	0.41
1:D:174:ILE:HD11	1:D:182:VAL:HG11	2.02	0.41
1:D:207:ALA:HB3	1:D:210:PRO:CG	2.51	0.41
1:D:297:THR:HB	1:D:300:LYS:H	1.86	0.41
1:D:131:LEU:HD11	1:D:147:ILE:CD1	2.51	0.40
1:A:49[A]:VAL:HG12	1:A:52:TYR:HB3	2.02	0.40
1:A:209:ALA:HB3	1:A:210:PRO:HD3	2.01	0.40
1:C:298:GLU:HA	1:C:299:HIS:HA	1.85	0.40
1:D:264:LEU:CD1	1:D:272:LEU:HD11	2.52	0.40
1:D:372:TYR:HA	1:D:375:THR:HG22	2.03	0.40
1:C:205:LEU:HD11	1:C:214:ALA:CB	2.52	0.40
1:B:375:THR:HG23	1:B:376:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/441 (93%)	404 (98%)	6 (2%)	1 (0%)	56	38
1	B	391/441 (89%)	374 (96%)	14 (4%)	3 (1%)	27	9
1	C	415/441 (94%)	404 (97%)	10 (2%)	1 (0%)	56	38
1	D	400/441 (91%)	384 (96%)	14 (4%)	2 (0%)	38	19
All	All	1617/1764 (92%)	1566 (97%)	44 (3%)	7 (0%)	43	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	VAL
1	C	343	VAL
1	D	343	VAL

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Mol	Chain	Res	Type
1	A	205	LEU
1	D	297	THR
1	B	242	GLY
1	B	173	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/368 (95%)	347 (99%)	3 (1%)	87	83
1	B	332/368 (90%)	329 (99%)	3 (1%)	87	83
1	C	351/368 (95%)	350 (100%)	1 (0%)	96	94
1	D	339/368 (92%)	336 (99%)	3 (1%)	87	83
All	All	1372/1472 (93%)	1362 (99%)	10 (1%)	91	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	102	PHE
1	A	170	ASN
1	B	102	PHE
1	B	172	PHE
1	B	266	ARG
1	C	102	PHE
1	D	1	MET
1	D	102	PHE
1	D	258	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	283	ASN
1	B	25	GLN

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Mol	Chain	Res	Type
1	B	319	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	411/441 (93%)	0.25	21 (5%) 27 21	24, 34, 60, 76	0
1	B	392/441 (88%)	0.35	33 (8%) 11 8	23, 35, 78, 89	0
1	C	411/441 (93%)	0.21	25 (6%) 21 15	25, 37, 58, 70	0
1	D	398/441 (90%)	0.32	44 (11%) 6 4	24, 37, 68, 86	0
All	All	1612/1764 (91%)	0.28	123 (7%) 14 10	23, 36, 66, 89	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	TYR	9.0
1	C	298	GLU	8.7
1	B	155	VAL	8.3
1	B	318	TYR	8.2
1	B	244	VAL	7.7
1	A	251	PRO	7.6
1	D	321	TRP	7.3
1	B	1	MET	6.7
1	A	245	TYR	6.7
1	D	157	ALA	6.6
1	C	269	ASP	6.0
1	A	-6	LEU	5.9
1	D	156	ASP	5.8
1	D	155	VAL	5.7
1	A	205	LEU	5.6
1	D	1	MET	5.6
1	C	321	TRP	5.4
1	B	154	ASP	5.4
1	B	319	GLN	5.3
1	C	346	THR	5.3
1	B	317	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	320	ALA	5.0
1	C	243	VAL	5.0
1	D	163	ILE	5.0
1	B	269	ASP	5.0
1	D	349	PHE	4.8
1	A	346	THR	4.8
1	A	244	VAL	4.8
1	C	299	HIS	4.7
1	B	316	ALA	4.6
1	B	251	PRO	4.6
1	C	244	VAL	4.5
1	B	255	GLU	4.5
1	C	313	ILE	4.4
1	C	-6	LEU	4.3
1	A	267	HIS	4.3
1	B	265	GLU	4.2
1	B	417	GLU	3.9
1	B	211	PHE	3.8
1	D	158	LYS	3.8
1	D	162	TYR	3.8
1	D	206	THR	3.8
1	D	159	THR	3.8
1	D	167	LEU	3.7
1	D	240	GLY	3.7
1	B	210	PRO	3.6
1	D	203	SER	3.6
1	D	255	GLU	3.6
1	B	256	TYR	3.5
1	B	227	ALA	3.5
1	D	333	GLU	3.5
1	A	266	ARG	3.5
1	D	51	ASP	3.5
1	D	261	LEU	3.4
1	A	243	VAL	3.4
1	A	343	VAL	3.4
1	D	161	PRO	3.3
1	B	266	ARG	3.3
1	D	343	VAL	3.2
1	D	164	SER	3.2
1	C	51[A]	ASP	3.2
1	A	333	GLU	3.2
1	C	252	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	LYS	3.2
1	A	334	ALA	3.2
1	B	250	PRO	3.2
1	A	-7	ASN	3.1
1	D	299	HIS	3.1
1	D	165	THR	3.1
1	D	350	LEU	3.1
1	B	202	GLY	3.1
1	B	267	HIS	3.0
1	D	205	LEU	2.9
1	D	254	SER	2.9
1	D	297	THR	2.8
1	C	331[A]	GLN	2.8
1	A	252	GLN	2.8
1	C	268	ARG	2.8
1	D	168	ARG	2.8
1	B	268	ARG	2.8
1	B	172	PHE	2.8
1	D	268[A]	ARG	2.7
1	D	313	ILE	2.7
1	A	297	THR	2.7
1	A	256	TYR	2.7
1	C	333	GLU	2.7
1	A	206	THR	2.7
1	B	321	TRP	2.6
1	D	417	GLU	2.6
1	D	256	TYR	2.6
1	B	177	ASP	2.6
1	D	52	TYR	2.6
1	C	300	LYS	2.5
1	C	314	ARG	2.5
1	D	204	GLN	2.5
1	B	333	GLU	2.5
1	C	349	PHE	2.5
1	D	160	HIS	2.5
1	D	169	ASP	2.5
1	C	206	THR	2.4
1	C	297	THR	2.4
1	A	227	ALA	2.4
1	D	154	ASP	2.4
1	C	417	GLU	2.4
1	D	211	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	217	ARG	2.3
1	B	51	ASP	2.3
1	C	255	GLU	2.3
1	B	213	ASP	2.3
1	D	258	LYS	2.3
1	D	177	ASP	2.2
1	B	258	LYS	2.2
1	B	313	ILE	2.2
1	D	266	ARG	2.2
1	C	241	LEU	2.2
1	C	240	GLY	2.2
1	A	32	VAL	2.1
1	C	177	ASP	2.1
1	C	169	ASP	2.1
1	D	298	GLU	2.0
1	B	262	ASP	2.0
1	A	347	SER	2.0
1	D	344	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	D	418	1/1	0.03	-1.67	42,42,42,42	0
2	CL	C	418	1/1	0.03	-2.52	38,38,38,38	0
2	CL	A	418	1/1	0.04	-2.80	44,44,44,44	0
2	CL	C	419	1/1	0.04	-3.41	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.